

Supporting Information for the Letter

“Electron Optics in Phosphorene pn Junctions: Negative Reflection and Anti-super-Klein Tunneling”

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In this supplementary material, we investigate electron optics in phosphorene pn junctions for lower electron energies, where the dispersion is quadratic in both directions. We demonstrate that the electron optics laws presented in the main article remain generally valid. In particular, negative reflection and anti-super-Klein tunneling can still be observed. Moreover, the electron optics laws in the low energy regime can be simplified even further leading to a single analytic expression.

ELECTRON OPTICS AT LOWER ENERGIES

The electron optics laws for phosphorene pn junctions, which are derived in the main text, are valid for all energies, where the dispersion relation in equation (4) holds. In Figures S1 and S2 we show these laws evaluated for electrons with energies $E = \Delta + 0.1 |t_1| \approx 1.1 |t_1|$ and $E = \Delta + 0.05 |t_1| \approx 1.05 |t_1|$, which are lower than in the main text. We find that the angle of reflection θ_r as a function of the angle of incidence θ_i changes only marginally if the electron energy is lowered. Most notably, negative reflection and anti-super Klein tunneling are preserved. The transmission curves and pseudo-spin differences decrease but keep their overall shape. All these observations are confirmed by the numerically calculated current flow patterns.

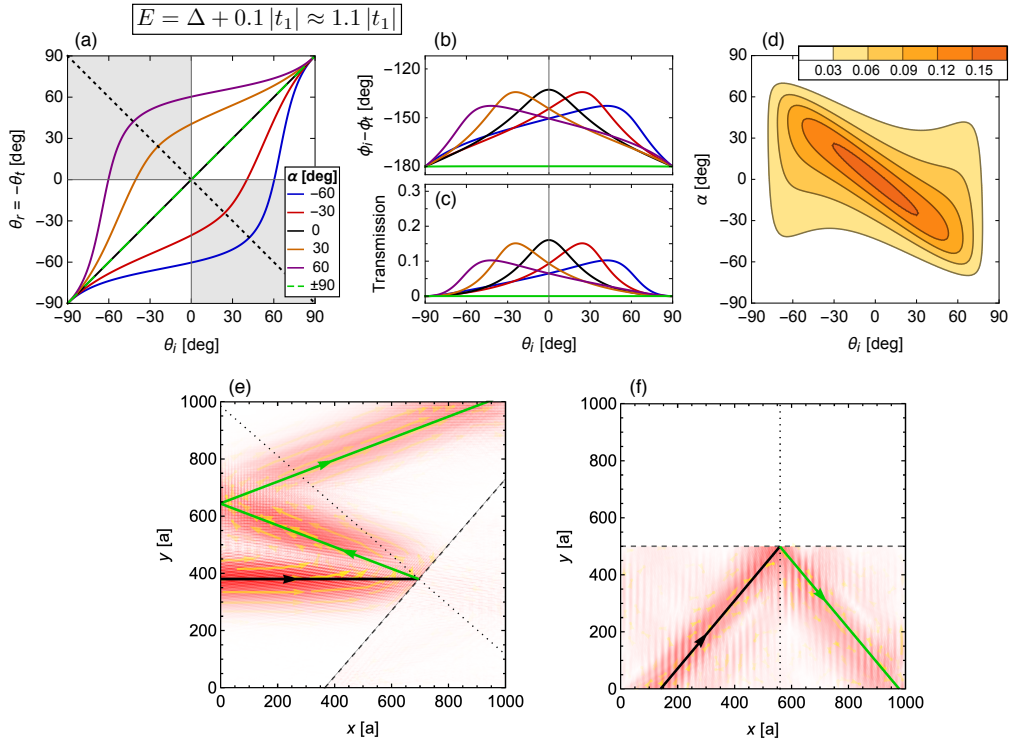


Figure S1. Electron optics laws in a phosphorene pn junction with $V = 2E$ and electrons with energy $E = \Delta + 0.1 |t_1| \approx 1.1 |t_1|$. (a) Reflection angle θ_r as a function of the incidence angle θ_i for various tilting angles α of the junction. (b) Difference of the pseudo-spins for the incident and transmitted electrons, $\phi_i - \phi_t$. (c,d) Transmission as a function of θ_i and α . (e,f) Numerically calculated current flow (red color shading, yellow arrows) and raylike electron trajectories of geometric optics (solid lines).

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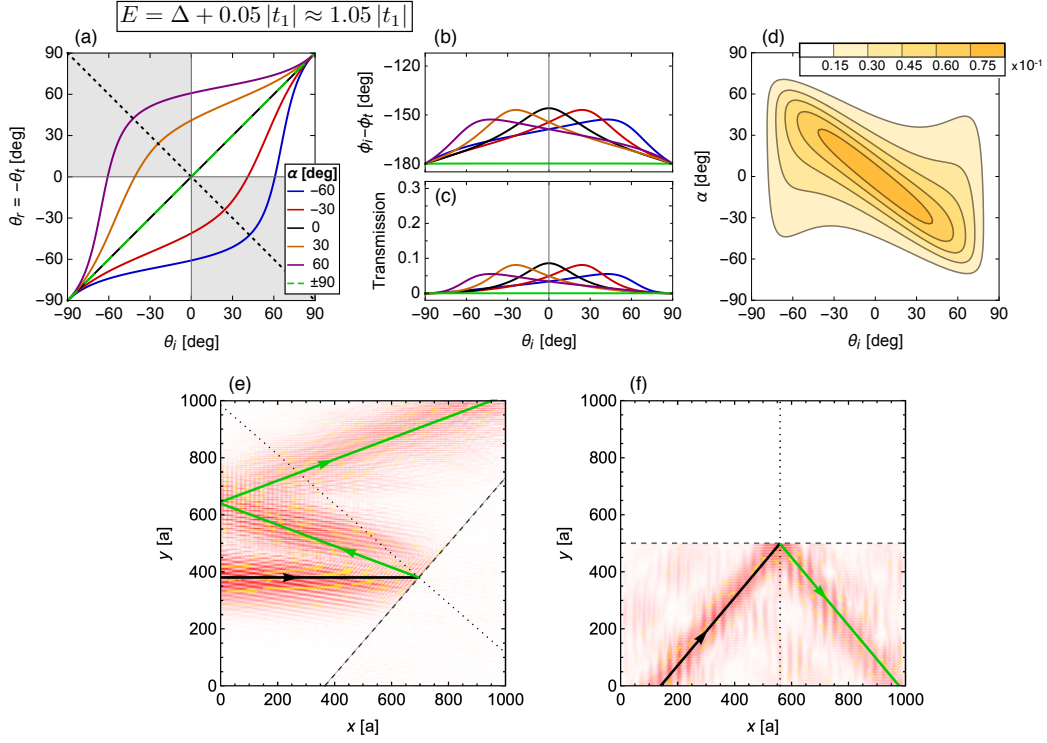


Figure S2. Electron optics in a phosphorene pn junction with $V = 2E$ for electrons with energy $E = \Delta + 0.05 |t_1| \approx 1.05 |t_1|$. The specification of the panels (a-f) is the same as in Figure S1.

At low energies the electron optics laws in phosphorene pn junctions can be simplified further by taking into account that the dispersion relation for such energies is quadratic in both directions

$$E = \sqrt{\left(\Delta + \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y}\right)^2 + \hbar^2 v^2 k_x^2} \approx \Delta + \frac{\hbar^2 k_x^2}{2\mu_x} + \frac{\hbar^2 k_y^2}{2m_y} \quad (\text{S.1})$$

with the effective mass $\mu_x = \frac{m_x}{1+m_x v^2/\Delta}$. This equation can also be written as

$$\frac{k_x^2}{l_x^2} + \frac{k_y^2}{l_y^2} = 1, \quad (\text{S.2})$$

where $l_x^2 = 2\mu_x(E - \Delta)/\hbar^2$ and $l_y^2 = 2m_y(E - \Delta)/\hbar^2$ are the squared lengths of the semi-axes of an ellipse. The straight blue-dashed line in Figure 2 (c) in the main text that connects the two regions can be parametrized by

$$k_y = k_x \tan \alpha + l_0, \quad (\text{S.3})$$

where l_0 is a constant. Its intersection points with the elliptical constant energy contours determine the wave vectors $\mathbf{k}_{i/r}$. Using these equations, we obtain the relation

$$k_{i,x} + k_{r,x} = -\frac{2l_0 \tan \alpha}{\rho + \tan^2 \alpha}, \quad (\text{S.4})$$

where $\rho = m_y/\mu_x$ is the mass ratio. The angles of incidence and reflection can be expressed in terms of $\mathbf{k}_i$ and $\mathbf{k}_r$ as

$$\tan \theta_i = \frac{v_{i,y}}{v_{i,x}} = \frac{-\frac{k_{i,x}}{\mu_x} \sin \alpha + \frac{k_{i,y}}{m_y} \cos \alpha}{\frac{k_{i,x}}{\mu_x} \cos \alpha + \frac{k_{i,y}}{m_y} \sin \alpha} = \frac{(1 - \rho) \tan \alpha + \frac{l_0}{k_{i,x}}}{\rho + \tan^2 \alpha + \frac{l_0}{k_{i,x}} \tan \alpha} \quad (\text{S.5})$$

and

$$\tan \theta_r = -\frac{v_{r,y}}{v_{r,x}} = \frac{\frac{k_{r,x}}{\mu_x} \sin \alpha - \frac{k_{r,y}}{m_y} \cos \alpha}{\frac{k_{r,x}}{\mu_x} \cos \alpha + \frac{k_{r,y}}{m_y} \sin \alpha} = \frac{(\rho - 1) \tan \alpha - \frac{l_0}{k_{r,x}}}{\rho + \tan^2 \alpha + \frac{l_0}{k_{r,x}} \tan \alpha}. \quad (\text{S.6})$$

We can eliminate from these equations the wave vector dependency by using the equations above and obtain finally for the reflection law in the low energy regime

$$\tan \theta_r = \tan \theta_i + 2 \tan \theta_b, \quad (\text{S.7})$$

with

$$\tan \theta_b = \frac{(\rho - 1) \tan \alpha}{\rho + \tan^2 \alpha}. \quad (\text{S.8})$$

θ_b is defined as the angle at which the incident electron beam is backscattered in the same direction ($\theta_r = -\theta_i$), see for example in Figure S1 (a) the intersection points of the black-dotted line with the colored curves. The reflection law in the low energy regime is shown in Figure S3 by means of the solid curves, while the general solution from the main text is shown by the dashed curves. Even for electrons with energy $E \approx 1.2 |t_1|$ the low energy approximation and the general solution agree very well (a). As expected, these differences decrease if the electron energy is lowered (b). For $\alpha = 0^\circ, \pm 90^\circ$, the conventional reflection law $\theta_r = \theta_i$ is recovered. Moreover, the equation (S.7) confirms our observation from Figures S1 and S2 that the reflection law at low energies is independent of the electron energy E .

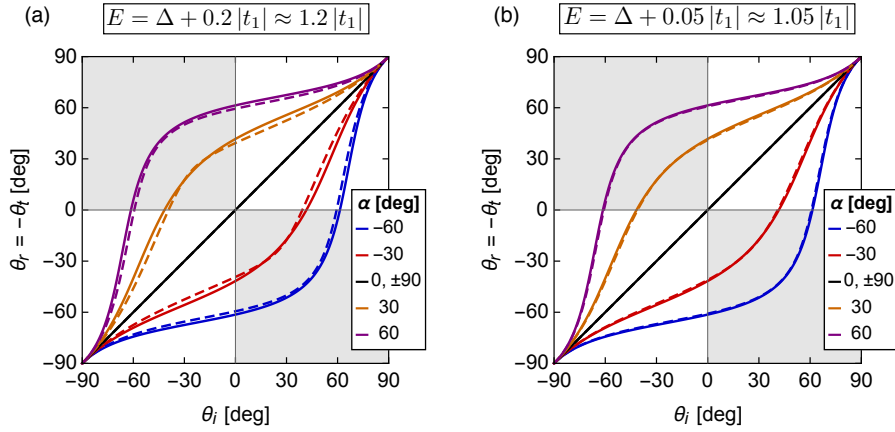


Figure S3. Electron reflection law in a phosphorene *pn* junction with $V = 2E$ and electrons with energy $E \approx 1.2 |t_1|$ (a) and $E \approx 1.05 |t_1|$ (b). The solid lines give the low energy approximation of equation (S.7), while the dashed lines are the general result from the main text. The curves show minor but visible differences, which decrease when the electron energy is lowered, compare (a) and (b).